

WHAT IS CLAIMED IS:

- 1 1. A method for screening potential catalysts for polymerization performance
2 comprising:
3 reacting a potential catalyst with at least a first monomer under polymerization
4 conditions;
5 determining the polymerization performance of the catalyst with the at least first
6 monomer; and
7 using the determination as a predictor for the polymerization performance of the
8 catalyst for at least a second monomer;
9 wherein the first and second monomers are different from each other and the first
10 monomer is an olefin other than ethylene.
- 1 2. A screening method according to Claim 1 wherein the step of using the
2 determination as a predictor comprises copolymerizing the first and second monomers
3 using the catalyst.
- 1 3. A screening method according to Claim 2 comprising copolymerizing the first
2 and second monomers in commercial quantities using the catalyst.
- 1 4. A screening method according to Claim 1 wherein the step of determining the
2 polymerization performance comprises measuring at least one property of the reaction
3 products.
- 1 5. A screening method according to Claim 1 wherein the step of using the
2 determination as a predictor comprises polymerizing at least the second monomer using
3 the catalyst.
- 1 6. A screening method according to Claim 1 wherein the step of determining the
2 polymerization performance comprises measuring the molecular weight of the polymer
3 formed under the polymerization conditions and using the catalyst.

1 7. A screening method according to Claim 1 wherein the step of determining the
2 polymerization performance comprises measuring the concentration of the polymer
3 formed under the polymerization conditions and using the catalyst.

1 8. A screening method according to Claim 1 wherein the step of determining the
2 polymerization performance comprises measuring the polydispersity index of the
3 polymer formed under the polymerization conditions and using the catalyst.

1 9. A screening method according to Claim 1 wherein the step of determining the
2 polymerization performance comprises analyzing the polymer using a high throughput
3 chromatography technique.

1 10. A screening method according to Claim 9 comprising analyzing the polymer
2 using size exclusion chromatography.

1 11. A screening method according to Claim 1 comprising reacting the potential
2 catalyst with a first monomer that is a liquid at room temperature and atmospheric
3 pressure.

1 12. A screening method according to Claim 1 comprising reacting the potential
2 catalyst with a monomer selected from the group consisting of 1-octene, 1-hexene, 1-
3 heptene, 1-nonene, and 1 decene.

1 13. A screening method according to Claim 1, wherein the second monomer is a
2 gas at room temperature and atmospheric pressure.

1 14. A screening method according to Claim 1, wherein the determination is used
2 as a predictor for the polymerization performance of the catalyst for a co-polymerization
3 of two or more monomers which include at least the first monomer.

1 15. A screening method according to Claim 1 wherein the step of reacting the
2 catalyst with the first monomer comprises reacting the catalyst with 1-octene; and

3 the step of using the determination as a predictor for a second monomer
4 comprises using the determination as a predictor for a monomer selected from the group
5 consisting of olefins lower in molecular weight than octene.

1 16. A method of screening potential catalysts for polymerization activity wherein
2 the polymerization activity of the potential catalysts is determined for at least a first
3 monomer as a predictor for the polymerization activity of the potential catalysts for at
4 least a second monomer, the first and second monomers being different from each other
and the first monomer being an olefin other than ethylene, the method comprising:

6 concurrently reacting an array of at least 8 potential polymerization catalysts that
7 are different from each other with at least a first monomer under polymerization
8 conditions; and

9 determining the polymerization performance of each of the potential catalysts
10 with the at least first monomer.

1 17. A screening method according to Claim 16 further comprising the step of
2 copolymerizing the first and second monomers using one of the catalysts in the array
3 based upon the polymerization performance of the catalyst.

1 18. A screening method according to Claim 17 comprising copolymerizing the
2 first and second monomers in commercial quantities.

1 19. A screening method according to Claim 16 wherein the step of determining
2 the polymerization performance comprises measuring a characteristic of the reaction
3 products.

1 20. A screening method according to Claim 16 further comprising the step of
2 polymerizing the at least second monomer using the catalyst.

1 21. A screening method according to Claim 20 comprising polymerizing the
2 second monomer in commercial quantities.

1 22. A screening method according to Claim 16 wherein the step of determining
2 the polymerization performance comprises analyzing the polymer using a high
3 throughput chromatography technique.

1 23. A screening method according to Claim 22 comprising analyzing the polymer
2 using size exclusion chromatography.

1 24. A screening method according to Claim 16, wherein the array of potential
2 catalysts comprises a substrate having wells with each of the at least 8 catalysts residing
3 in a different well of the substrate.

1 25. A screening method according to Claim 16, wherein the reacting step further
2 comprises adding other compositions to the wells other than the first or second monomers
3 or the catalysts.

1 26. A screening method according to Claim 16 comprising dispensing the first
2 monomer as a liquid into each reaction vessel that contains one of the potential catalysts
3 prior to the step of reacting the catalyst with the first monomer.

1 27. A screening method according to Claim 16 comprising distributing the first
2 monomer as a gas to each reaction vessel that contains one of the potential catalysts prior
3 to the step of reacting the catalyst with the first monomer.

1 28. A screening method according to Claim 16 further comprising:
2 activating the potential catalysts; and
3 wherein at least a portion of the at least first monomer is provided to each reaction
4 vessel prior to activation of the potential catalysts.

1 29. A screening method according to Claim 16, wherein the step of determining
2 the polymerization performance of the catalysts comprises measuring a property of any
3 polymer sample made during the reaction step, wherein the property is selected from the
4 group consisting of molecular weight, polydispersity index, viscosity, concentration,

5 solvent extractables, solubility, melt flow index, glass transition temperature, melting
6 point, percent crystallinity, density, polymer mass, polymer composition, polymer
7 structure, polymer architecture, and combinations thereof.

1 30. A screening method according to Claim 16, wherein the determination of
2 polymerization performance comprises measuring a property of the reaction mixture from
3 any members of the array, wherein the property is selected from the group consisting of
4 monomer concentration, monomer conversion, ratio of catalyst to monomer, light
5 scattering, viscosity, temperature, visual inspection, intrinsic viscosity, polymer
6 concentration, molecular weight, and combinations thereof.

1 31. A screening method according to Claim 16, wherein the reacting step is
2 carried out to a predetermined point selected from the group consisting of time, monomer
3 consumption, heat of reaction, polymer concentration, viscosity, and molecular weight.

1 32. A screening method according to Claim 31 and further comprising quenching
2 the reaction at the predetermined point.

1 33. A screening method according to Claim 16, wherein the reacting step
2 comprises concurrently reacting all potential catalysts in the array with the first
3 monomer.

1 34. A screening method according to Claim 16, wherein the determination is used
2 as a predictor for the polymerization activity of the potential catalysts for a co-
3 polymerization of the second monomer with a third monomer.

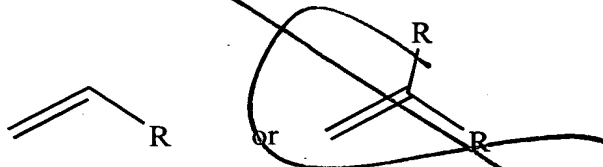
1 35. A screening method according to Claim 34 and further comprising the step of
2 copolymerizing the second and third monomers.

1 36. A screening method according to Claim 35 comprising copolymerizing the
2 second and third monomers in commercial quantities.

1 37. A method according to Claim 16 wherein the first monomer is an α -olefin.

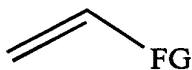
1 38. A method according to Claim 37 wherein the first monomer is selected from
2 the group consisting of 1-octene, 1-hexene, 1-heptene, 1-nonene, and 1 decene.

3
4 39. A screening method according to Claim 14, wherein the at least first
5 monomer is an α -olefin represented by either formula:



7 wherein each R is independently selected from the group consisting of halogen, alkyl,
8 substituted alkyl, aryl, substituted aryl, heteroalkyl, cycloalkyl, substituted cycloalkyl,
9 heterocycloalkyl, substituted heterocycloalkyl, heteroaryl, substituted heteroaryl, alkoxy,
10 silyl, boryl, phosphino, amino, thio, seleno and combinations thereof.

1 40. A screening method according to Claim 16 wherein at least the first monomer
2 is represented by the formula:



wherein FG is a halogen or a functional group that contains at least one heteroatom.

1 41. A screening method according to Claim 16 comprising:
2 measuring the polymerization activity of each of the potential catalysts with the at
3 least first monomer; and
4 predicting the polymerization activity of each of the potential catalysts for at least
5 a second monomer, wherein the first and second monomers are chemically different from
each other and the first monomer is an olefin other than ethylene.

1 42. A screening method for high throughput screening of potential catalysts for
2 polymerization activity for at least a second monomer, comprising:
3 concurrently reacting a plurality of at least 8 potential catalysts arrayed on a
4 substrate with a first monomer; and

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determining a property of any polymer sample or polymerization mixture made during the reaction step at a rate of one hour or less per potential catalyst.

1 43. A screening method according to Claim 42 comprising:
2 concurrently reacting at least 24 potential catalysts; and
3 determining properties at a rate of about 20 minutes or less per potential catalyst.

1 44. A screening method according to Claim 42 wherein the step of determining
2 the polymerization performance comprises measuring a characteristic of the reaction
3 products.

1 45. A screening method according to Claim 42 wherein the step of determining a
2 property comprises measuring the concentration of the polymer formed using the catalyst.

1 46. A screening method according to Claim 42 wherein the step of determining a
2 property comprises measuring the polydispersity index of the polymer formed using the
3 catalyst.

1 47. A screening method according to Claim 42 wherein the step of determining a
2 property comprises analyzing the polymer using a high throughput chromatography
3 technique.

1 48. A screening method according to Claim 47 comprising analyzing the polymer
2 using size exclusion chromatography.

1 49. A screening method according to Claim 42, wherein the step of determining a
2 property comprises measuring a property of any polymer sample made during the
3 reaction step, wherein the property is selected from the group consisting of molecular
4 weight, polydispersity index, viscosity, concentration, solvent extractables, solubility,
5 melt flow index, glass transition temperature, melting point, percent crystallinity, density,
6 polymer mass, polymer composition, polymer structure, polymer architecture, and
7 combinations thereof.

1 50. A screening method according to Claim 42, wherein the step of determining a
2 property comprises measuring a property of the polymerization reaction mixture from
3 any members of the array, wherein the property is selected from the group consisting of
4 monomer concentration, monomer conversion, ratio of catalyst to monomer, light
5 scattering, viscosity, temperature, visual inspection, intrinsic viscosity, polymer
6 concentration, molecular weight, and combinations thereof.

1 51. A screening method according to Claim 42, wherein the concurrent reactions
2 are carried out to a predetermined point selected from the group consisting of time,
3 monomer consumption, heat of reaction, polymer concentration, viscosity, and molecular
4 weight.

1 52. A screening method according to Claim 51 and further comprising
2 concurrently quenching the reaction at the predetermined point.

1 53. A screening method according to Claim 42, wherein the determination is used
2 as a predictor for the polymerization activity of the potential catalysts for a co-
3 polymerization of the second monomer with at least a third monomer.

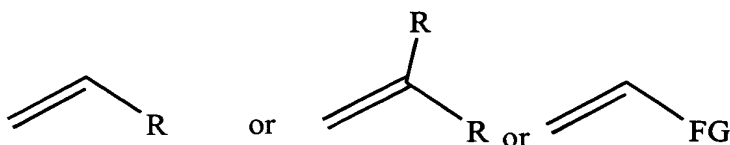
1 54. A screening method according to Claim 53 and further comprising the step of
2 copolymerizing the at least second and third monomers.

1 55. A screening method according to Claim 54 comprising copolymerizing the at
2 least second and third monomers in commercial quantities.

1 56. A method according to Claim 42 wherein the first monomer is an olefin other
2 than ethylene.

1 57. A method according to Claim 42 wherein the first monomer is 1-octene, 1-
2 hexene, 1-heptene, 1-nonene, and 1 decene.

1 58. A screening method according to Claim 41, wherein the first monomer is
2 represented by a formula selected from the group consisting of:



4 wherein each R is independently selected from the group consisting of halogen, alkyl,
5 substituted alkyl, aryl, substituted aryl, heteroalkyl, cycloalkyl, substituted cycloalkyl,
6 heterocycloalkyl, substituted heterocycloalkyl, heteroaryl, substituted heteroaryl, alkoxy,
7 sityl, boryl, phosphino, amino, thio, seleno and combinations thereof; and FG is halogen
8 or a functional group that contains at least one heteroatom.

1 59. A method for high throughput screening of potential catalysts for
2 polymerization activity for at least a second monomer, comprising:
3 combining a plurality of catalysts with an array of portions of a first monomer,
4 with the number of portions of monomers being greater than the number of catalysts, and
5 with no more than one catalyst in each of the monomer portions;
6 concurrently initiating a polymerization reaction in each of the monomer portions;
7 concurrently quenching the polymerization reaction in each of the monomer
8 portions; and
9 sampling the portions at a rate of between about 30 seconds and eight minutes per
10 sample.

1 60. A screening method according to Claim 59 comprising combining the
2 plurality of catalyst with 96 portions of the first monomer.

1 61. A screening method according to Claim 59, wherein the step of sampling the
2 portions comprises determining a property of the sample selected from the group
3 consisting of polymer properties and polymerization mixture properties.

1 62. A screening method according to Claim 59 and further comprising the step of
2 combining ligands and metal precursors to form the catalysts prior to the step of
3 combining the catalysts with the monomer portions.

1 63. A screening method according to Claim 62 further comprising combining the
2 catalysts with one or more activators.

1 64. A catalyst library comprising:
2 a plurality of compounds;
3 a benchmark quality of polymerization of a particular olefin; and
4 the information as to whether each compound falls above or below the olefin-
5 polymerization benchmark.

01 65. A catalyst library comprising:
02 a plurality of compounds;
03 a benchmark quality of the polymerization of 1-octene; and
04 the information as to whether each compound falls above or below the octene
05 polymerization benchmark.

01 66. A catalyst library according to Claim 65 wherein the benchmark quality is
02 selected from the group consisting of: molecular weight, polymerization rate, viscosity,
03 concentration, solvent extractables, solubility, melt flow index, glass transition
04 temperature, melting point, percent crystallinity, density, polymer mass, polymer
5 composition, polymer structure, polymer architecture, monomer concentration, monomer
6 conversion, ratio of catalyst to monomer, light scattering, viscosity, temperature, visual
7 inspection, intrinsic viscosity, polymer concentration, molecular weight, and
8 combinations thereof.

1 67. A method of producing a benchmark library for the polymerization of olefins
2 comprising screening a plurality of catalysts against the benchmark at a rate of between
3 about 30 seconds and 20 minutes per catalyst.

1 68. The method of claim 67, wherein the rate is between about 30 seconds and 10
2 minutes.

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1 69. The method of claim 68 wherein the rate is between about 30 seconds and
2 8minutes.

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